Bromoacetic acid, 2-naphthyl ester

Inchi: InChI=1S/C12H9BrO2/c13-8-12(14)15-11-6-5-9-3-1-2-4-10(9)7-11/h1-7H,8H2
InchiKey: XJWDIZWNDCUOMG-UHFFFAOYSA-N
Formula: C12H9BrO2
SMILES: O=C(CBr)Oc1ccc2ccccc2c1
Mol. weight [g/mol]: 265.10

Physical Properties

Property code	Value	Unit	Source
gf	39.99	kJ/mol	Joback Method
hf	-93.35	kJ/mol	Joback Method
hfus	25.58	kJ/mol	Joback Method
hvap	62.48	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.140		Crippen Method
mcvol	161.660	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	667.05	K	Joback Method
tc	914.19	K	Joback Method
tf	428.60	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.47	J/mol×K	667.05	Joback Method
cpg	382.23	J/mol×K	708.24	Joback Method
cpg	393.04	J/mol×K	749.43	Joback Method
cpg	402.97	J/mol×K	790.62	Joback Method
cpg	412.09	J/mol×K	831.81	Joback Method
cpg	420.49	J/mol×K	873.00	Joback Method
cpg	428.25	J/mol×K	914.19	Joback Method
dvisc	0.0013275	Pa×s	428.60	Joback Method

dvisc	0.0009336	Pa×s	468.34	Joback Method
dvisc	0.0006937	Pa×s	508.08	Joback Method
dvisc	0.0005382	Pa×s	547.83	Joback Method
dvisc	0.0004321	Pa×s	587.57	Joback Method
dvisc	0.0003567	Pa×s	627.31	Joback Method
dvisc	0.0003013	Pa×s	667.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308052&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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